

LAPLACIAN ESTRADA INDEX OF TREES

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Abstract

Let G be a simple graph with n vertices and let $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} \geq \mu_n = 0$ be the eigenvalues of its Laplacian matrix. The Laplacian Estrada index of a graph G is defined as $LEE(G) = \sum_{i=1}^n e^{\mu_i}$. Using the recent connection between Estrada index of a line graph and Laplacian Estrada index, we prove that the path P_n has minimal, while the star S_n has maximal LEE among trees on n vertices. In addition, we find the unique tree with the second maximal Laplacian Estrada index.

1. INTRODUCTION

Let G be a simple graph with n vertices. The spectrum of G consists of the eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ of its adjacency matrix [1]. The Estrada index of G

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is defined as

$$EE(G) = \sum_{i=1}^n e^{\lambda_i}. \quad (1)$$

This graph-spectrum-based graph invariant was put forward by Estrada in [2, 3], where it was shown that $EE(G)$ can be used as a measure of the degree of folding of long chain polymeric molecules. Further, it was shown in [4] that the Estrada index provides a measure of the centrality of complex networks, while a connection between the Estrada index and the concept of extended atomic branching was pointed out in [5]. Some mathematical properties of the Estrada index were studied in [6]–[16].

For a graph G with n vertices, let $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} \geq \mu_n = 0$ be the eigenvalues of its Laplacian matrix [17]. In full analogy with Equation (1), the Laplacian Estrada index of G is defined as [18]

$$LEE(G) = \sum_{i=1}^n e^{\mu_i}.$$

Bounds for the Laplacian Estrada index may be found in [18]–[20].

Let $\mathcal{L}(G)$ be the line graph of G . In [20], the authors proved the following relation between Laplacian Estrada index of G and Estrada index of a line graph of G .

Theorem 1. [20] *Let G be a graph with n vertices and m edges. If G is bipartite, then*

$$LEE(G) = n - m + e^2 \cdot EE(\mathcal{L}(G)).$$

Our goal here is to add some further evidence to support the use of LEE as a measure of branching in alkanes. While the measure of branching cannot be formally defined, there are several properties that any proposed measure has to satisfy [21, 22]. Basically, a topological index TI acceptable as a measure of branching must satisfy the inequalities

$$TI(P_n) < TI(T) < TI(S_n) \quad \text{or} \quad TI(P_n) > TI(T) > TI(S_n),$$

for $n = 5, 6, \dots$, where P_n is the path, S_n is the star on n vertices, and T is any n -vertex tree, different from P_n and S_n . For example, the first relation is obeyed by the largest graph eigenvalue [23] and Estrada index [14], while the second relation is obeyed by the Wiener index [24], Hosoya index and graph energy [25].

We show that among the n -vertex trees, the path P_n has minimal and the star S_n maximal Laplacian Estrada index,

$$LEE(P_n) < LEE(T) < LEE(S_n),$$

where T is any n -vertex tree, different from P_n and S_n . We also find the unique tree with the second maximal Laplacian Estrada index.

2. LAPLACIAN ESTRADA INDEX OF TREES

In our proofs, we will use a connection between Estrada index and the spectral moments of a graph. For $k \geq 0$, we denote by M_k the k th spectral moment of G ,

$$M_k = M_k(G) = \sum_{i=1}^n \lambda_i^k.$$

A walk of length k in G is any sequence of vertices and edges of G ,

$$w_0, e_1, w_1, e_2, \dots, w_{k-1}, e_k, w_k,$$

such that e_i is the edge joining w_{i-1} and w_i for every $i = 1, 2, \dots, k$. The walk is closed if $w_0 = w_k$. It is well-known (see [1]) that $M_k(G)$ represents the number of closed walks of length k in G . Obviously, for every graph $M_0 = n$, $M_1 = 0$ and $M_2 = 2m$. From the Taylor expansion of e^x , we have that the Estrada index and the spectral moments of G are related by

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k}{k!}. \quad (2)$$

Thus, if for two graphs G and H we have $M_k(G) \geq M_k(H)$ for all $k \geq 0$, then $EE(G) \geq EE(H)$. Moreover, if the strict inequality $M_k(G) > M_k(H)$ holds for at least one value of k , then $EE(G) > EE(H)$.

Among the n -vertex connected graphs, the path P_n has minimal and the complete graph K_n maximal Estrada index [8, 14],

$$EE(P_n) < EE(G) < EE(K_n), \quad (3)$$

where G is any n -vertex connected graph, different from P_n and K_n .

Theorem 2. *Among the n -vertex trees, the path P_n has minimal and the star S_n maximal Laplacian Estrada index,*

$$LEE(P_n) < LEE(T) < LEE(S_n),$$

where T is any n -vertex tree, different from P_n and S_n .

Proof. The line graph of a tree T is a connected graph with $n - 1$ vertices. The line graph of a path P_n is also a path P_{n-1} , while the line graph of a star S_n is a complete graph K_{n-1} . Using the relation (3) it follows that

$$EE(\mathcal{L}(P_n)) \leq EE(\mathcal{L}(T)) \leq EE(\mathcal{L}(S_n)),$$

and from Theorem 1 we get $LEE(P_n) \leq LEE(T) \leq LEE(S_n)$ with left equality if and only if $T \cong P_n$ and right equality if and only if $T \cong S_n$. \square

3. SECOND MAXIMAL LAPLACIAN ESTRADA OF TREES

Definition 1. Let v be a vertex of degree $p + 1$ in a graph G , which is not a star, such that vv_1, vv_2, \dots, vv_p are pendent edges incident with v and u is the neighbor of v distinct from v_1, v_2, \dots, v_p . We form a graph $G' = \sigma(G, v)$ by removing edges vv_1, vv_2, \dots, vv_p and adding new edges uv_1, uv_2, \dots, uv_p . We say that G' is σ -transform of G .

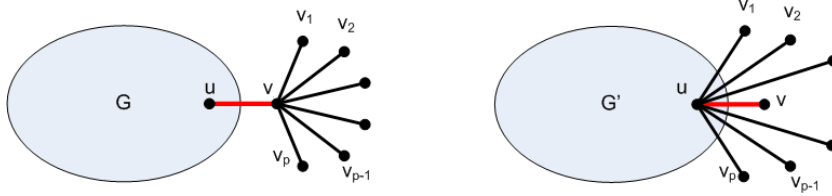


Figure 1: σ -transformation applied to G at vertex v .

Theorem 3. Let $G' = \sigma(G, v)$ be a σ -transform of a bipartite graph G . Then

$$LEE(G) < LEE(G'). \quad (4)$$

Proof. The graphs G and G' are both bipartite and have the same number of vertices and edges. Using Theorem 1, it is enough to prove inequality

$$EE(\mathcal{L}(G)) < EE(\mathcal{L}(G')).$$

Let u_1, u_2, \dots, u_m be the neighbors of u in G , different from v . Consider the induced subgraph H of $\mathcal{L}(G)$ formed using vertices $vv_1, vv_2, \dots, vv_p, vu, uu_1, uu_2, \dots, uu_m$. It is easy to see that these vertices are grouped in two cliques of sizes $p + 1$ and $m + 1$ with the vertex uv in common. Similarly, consider the induced subgraph H' of $\mathcal{L}(G')$

formed using corresponding vertices $uv_1, uv_2, \dots, uv_p, vu, uu_1, uu_2, \dots, uu_m$. Here, we have one clique of size $m + p + 1$.

Since H is a proper subgraph of H' , it follows that for every $k \geq 0$, $M_k(H') \geq M_k(H)$ and then $M_k(\mathcal{L}(G')) \geq M_k(\mathcal{L}(G))$, which is strict for some k . Finally, using the relation (2), we have $LEE(G) < LEE(G')$. \square

Let T be an arbitrary tree on n vertices with root v . We can find a vertex u that is the parent of the leaf on the deepest level and apply σ -transformation at u to strictly increase the Laplacian Estrada index.

Corollary 1. *Let T be a tree on n vertices. If $T \not\cong S_n$, then $LEE(T) < LEE(S_n)$.*

Let $S_n(a, b)$ be the tree formed by adding an edge between the centers of the stars S_a and S_b , where $a + b = n$ and $2 \leq a \leq \lfloor \frac{n}{2} \rfloor$. We call $S_n(a, b)$ the double star. By direct calculation, the characteristic polynomial of the Laplacian matrix of the double star $S_n(a, b)$ is equal to

$$P(x) = (-1)^n x(x-1)^{n-4} (x^3 - (n+2)x^2 + (n+2+ab)x - n).$$

We may assume that $n > 5$. The Laplacian spectra of $S_n(a, b)$ consists of three real roots of polynomial $f_{n,a}(x) = x^3 - (n+2)x^2 + (n+2+a(n-a))x - n$, 1 with multiplicity $n-4$, and 0 with multiplicity one. In order to establish the ordering of double stars with n vertices by LEE values it is enough to consider the following function $g_{n,a}(x_1, x_2, x_3) = e^{x_1} + e^{x_2} + e^{x_3}$, where $x_1 \geq x_2 \geq x_3 > 0$ are the roots of $f_{n,a}(x)$.

We locate x_1, x_2 and x_3 . First we have

$$f_{n,a}(n-a+1) = 1-a < 0$$

and

$$f_{n,a}\left(n-a+\frac{3}{2}\right) = \frac{15}{8} + a^2 + n + \frac{n^2}{2} - \frac{11a}{4} - \frac{3na}{2}.$$

The last function (considered as a quadratic function of a) is decreasing for $a < \frac{11}{8} + \frac{3n}{4}$, and then for $a \leq \frac{n}{2} - 1$, we have

$$f_{n,a}\left(n-a+\frac{3}{2}\right) \geq f_{n,a}\left(n-\frac{n}{2}+1+\frac{3}{2}\right) = \frac{45+n}{8} > 0.$$

Next we have

$$f_{n,a}(a) = (a-1)(n-2a) \geq 0 \quad \text{and} \quad f_{n,a}(a+1) = 1+a-n < 0.$$

Finally we have

$$f_{n,a}(0) = -n < 0 \quad \text{and} \quad f_{n,a}(1) = (a-1)(n-1-a) > 0.$$

Thus $x_3 \in [0, 1]$, $x_2 \in [a, a+1]$ and $x_1 \in [n-a+1, n-a+\frac{3}{2}]$ for $2 \leq a \leq \frac{n}{2} - 1$.

The function

$$h(a) = e^0 + e^a + e^{n-a+1} - e^1 - e^{a+2} - e^{n-a+1/2}$$

is decreasing for $a > 0$ (since $h'(a) < 0$), and then for $a \leq \frac{n}{2} - 1$ we have

$$h(a) \geq h\left(\frac{n}{2} - 1\right) = e^{n/2} (e^{-1} - e + e^2 - e^{3/2}) + 1 - e > \frac{e^{n/2}}{2} + 1 - e > 0.$$

Thus, for $2 \leq a < \lfloor \frac{n}{2} \rfloor - 1$, we have

$$e^0 + e^a + e^{n-a+1} > e^1 + e^{a+2} + e^{n-a+1/2},$$

and then $LEE(S_n(a, b)) > LEE(S_n(a+1, b-1))$. The special case $a = \lfloor \frac{n}{2} \rfloor$ can be handled easily,

$$\begin{aligned} & LEE(S_n(2, n-2)) - LEE\left(S_n\left(\left\lfloor \frac{n}{2} \right\rfloor, \left\lceil \frac{n}{2} \right\rceil\right)\right) \\ & > e^{n-1} + e^2 - e^{\lceil n/2 \rceil} - e^{\lceil n/2 \rceil + 2} - e > e^{\lceil n/2 \rceil} \cdot (e^{\lceil n/2 \rceil - 1} - 1 - e^2) - e > 0 \text{ for } n > 7 \end{aligned}$$

and by direct calculation, we also have $LEE(S_n(2, n-2)) - LEE(S_n(\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil)) > 0$ for $n = 6, 7$. By Theorem 3, the second maximal LEE for n -vertex trees is a double star $S_n(a, b)$, and then from discussions above, we have

Corollary 2. *The unique tree on $n \geq 5$ vertices with the second maximal Laplacian Estrada index is a double star $S_n(2, n-2)$.*

Note that as above, $LEE(S_n(3, n-3)) - LEE(S_n(\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil)) > 0$ for $n \geq 8$ (the cases for $n = 8, 9$ need direct calculation). Tested by computer on trees with at most 22 vertices, $S_n(3, n-3)$ is the unique tree with the third and $C_n(n-5)$ (formed by attaching $n-5$ vertices to the center of a path P_5) is the unique tree with the fourth maximal Laplacian Estrada index for $n \geq 6$.

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